SEARCH REQUEST FORM

Requestor's Name: Don Daus Serial Number: 405120

Date: 2 NOV 95 Phone: 4720 Art Unit: 1202

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s):

Please search structures of claims 1, 22-4

PCT/US 94/10530 probably has published (number not known yet)

need something besides that

Thanks

STAFF USE ONLY

Date completed: 11-03-95
Searcher: Beverly @ 4999
Terminal time: 45
Elapsed time: _____
CPU time: _____
Total time: 57
Number of Searches: _____
Number of Databases: 1

Search Site

_____ STIC
_____ CM-1
_____ Pre-S

Type of Search

_____ N.A. Sequence
_____ A.A. Sequence
_____ Structure
_____ Bibliographic

Vendors

_____ IG Suite
✓ STN
_____ Dialog
_____ APS
_____ Geninfo
_____ SDC
_____ DARC/Questel
_____ Other

Daus
405120

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=> fil reg; d que stat l6; fil marpat; d que stat l7; d l7 1-7 .bevmar;
fil marpatprev
FILE 'REGISTRY' ENTERED AT 12:49:41 ON 03 NOV 95
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STRUCTURE FILE UPDATES:  27 OCT 95   HIGHEST RN 169435-71-6
DICTIONARY FILE UPDATES:  2 Nov 95   HIGHEST RN 169435-71-6

TSCA INFORMATION NOW CURRENT THROUGH JUNE 1995

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.
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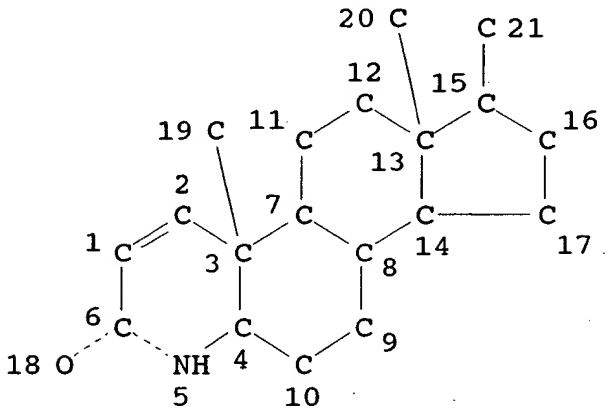

STYs. claims 22-24

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  21

STEREO ATTRIBUTES: NONE
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L5              STR
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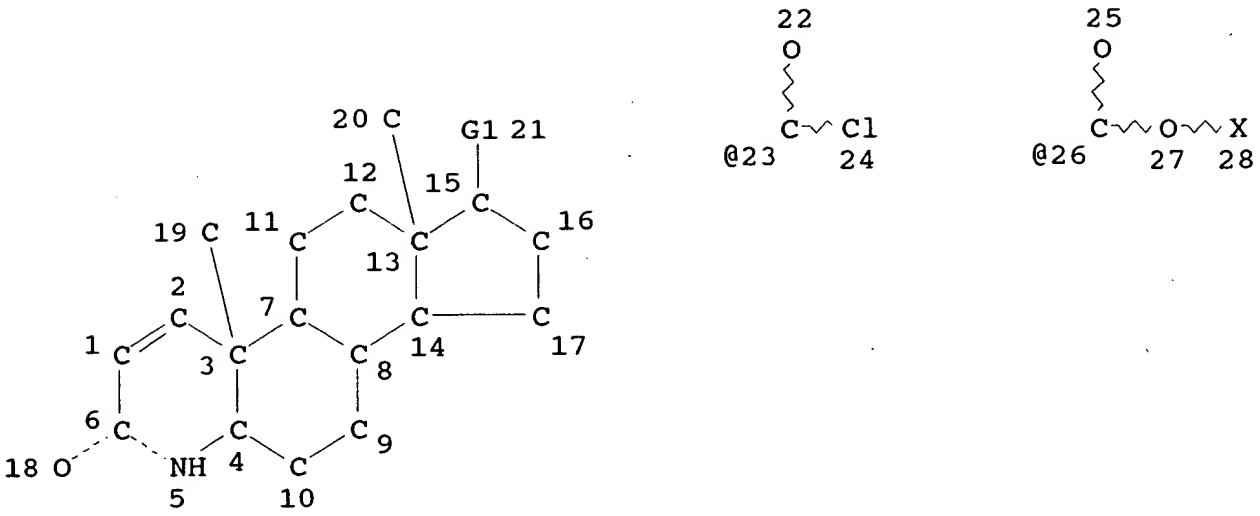


VAR G1=23/26
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE
L6 0 SEA FILE=REGISTRY SUB=L4 SSS FUL L5

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.09

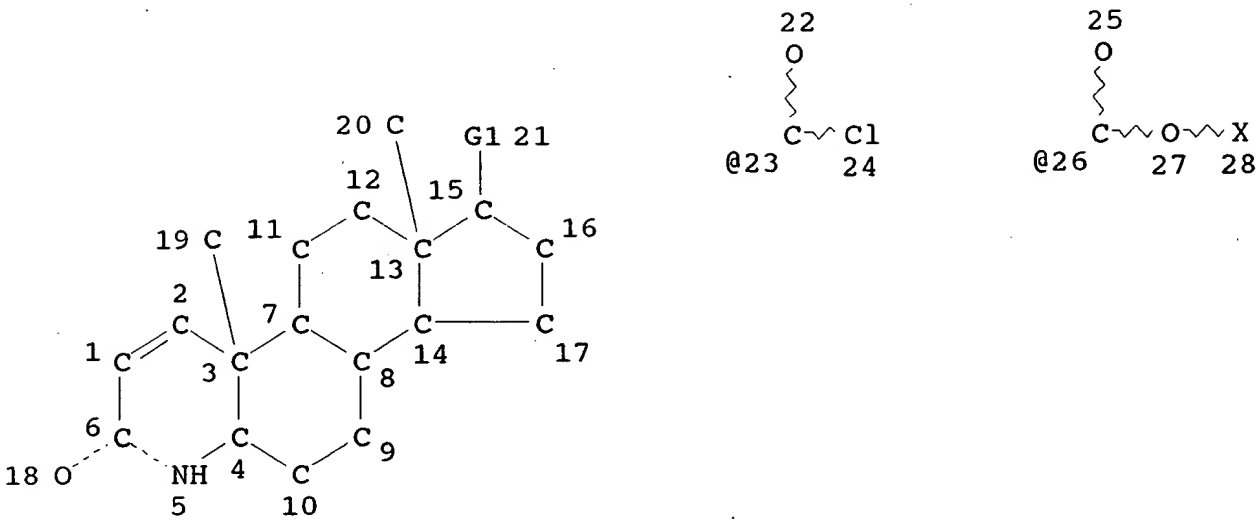
FILE 'MARPAT' ENTERED AT 12:49:43 ON 03 NOV 95

FILE CONTENT: 1988-1994 (VOL 108 ISS 14 - VOL 123 ISS 17) (951020 ED)

MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US	5441727	15 Aug 1995
DE	4407141	9 Sep 1995
EP	669131	30 Aug 1995
JP	07192868	28 Jul 1995
WO	9522171	17 Aug 1995

L5 STR



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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:
ECLEVEL IS LIM ON ALL NODES
ALL RING(S) ARE ISOLATED

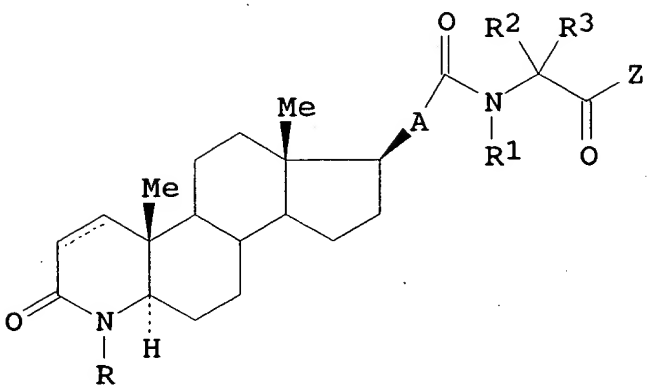
L7 7 SEA FILE=MARPAT SSS FUL L5 (MODIFIED ATTRIBUTES)

100.0% PROCESSED 24 ITERATIONS (2 INCOMPLETE) 7 ANSWERS
SEARCH TIME: 00.00.18

L7 ANSWER 1 OF 7 MARPAT COPYRIGHT 1995 ACS
AN 121:134563 MARPAT
TI 17.beta.-Substituted 4-aza-5.alpha.-androstan-3-one derivatives useful as testosterone 5.alpha.-reductase inhibitors, and their preparation, compositions, and use
IN Panzeri, Achille; Nesi, Marcella; Di, Salle Enrico
PA Farmitalia Carlo Erba S.R.L., Italy
SO PCT Int. Appl., 70 pp.
CODEN: PIXXD2
PI WO 9403476 A1 940217
DS W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP,

KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 93-EP2038 930729
PRAI GB 92-16329 920731
DT Patent
LA English
GI



I

AB Title compds. I [R = H, C1-C4 (fluoro)alkyl; A = bond, straight or branched C1-C6 alkylene chain; R1 = H, C1-C6 (fluoro)alkyl; R2 = (un)substituted C1-C6 alkyl, C5-C7 (fluoro)cycloalkyl, C6-C10 (fluoro)cycloalkylalkyl, (un)substituted aryl or C7-C10 arylalkyl, C6-C10 (fluoro)heterocycloalkyl; R3 = H, C1-C4 alkyl, (un)substituted aryl or C7-C10 arylalkyl; Z = C1-C6 (fluoro)alkyl, OR5 (wherein R5 = C1-C6 alkyl), NR6R7 (wherein R6, R7 = H, C1-C6 alkyl, C5-C7 cycloalkyl, Ph; or NR6R7 = 5- or 6-membered satd. heteromonocyclic ring); dotted line = optional pi bond; provided that R2 .noteq. unsubstituted alkyl when A = OR5] are testosterone 5.alpha.-reductase inhibitors, and are therapeutically useful in benign prostatic hyperplasia, prostatic and breast cancers, seborrhea, female hirsutism, and male pattern baldness. For example, D,L-alanine was converted in 5 steps to MeCH(NH2)CH(OH)CF3.HCl, obtained as a mixt. of both diastereomeric pairs. Amidation of this with 2-pyridyl 3-oxo-4-aza-5.alpha.-androst-1-ene-17.beta.-carbothioate, and Swern oxidn. of the sidechain hydroxyl group in the product, gave an epimeric mixt. of (22R,S)-I [R = R1 = R3 = H, R2 = Me, Z = CF3, A = bond, .DELTA.1 present] (II). At 3 mg/kg/day p.o. in castrated, androgen-replaced rats, II gave 58% inhibition of testosterone-induced prostatic hypertrophy. Twelve synthetic examples cover a variety of I epimers and epimeric mixts., and a list of 27 I with unspecified epimeric stereochem. is also claimed. Three pharmaceutical formulation examples are given.

IC ICM C07J073-00
ICS A61K031-58
CC 32-4 (Steroids)
Section cross-reference(s): 1, 2
ST azaandrostanone prepn testosterone reductase inhibitor; androstanone aza prepn testosterone reductase inhibitor; antiandrogen azaandrostenone prepn
IT Neoplasm inhibitors
(antiandrogenic azaandrostanone derivs.)
IT Hirsutism
(female, treatment of, azaandrostanone derivs. for)
IT Acne
Seborrhea
(treatment of, azaandrostanone derivs. for)
IT Steroids, preparation
RL: PREP (Preparation)
(4-aza-, oxo, azaandrostanone derivs., as 5.alpha.-reductase inhibitors)
IT Androgens
RL: RCT (Reactant)
(antiandrogens, azaandrostanone derivs.)
IT Prostate gland
(disease, benign hyperplasia, treatment of, azaandrostanone derivs. for)
IT Alopecia
(male pattern, treatment of, azaandrostanone derivs. for)
IT Mammary gland
Prostate gland
(neoplasm, treatment of, azaandrostanone derivs. for)
IT 156990-63-5 156990-64-6
RL: RCT (Reactant)
(Grignard reaction of, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)
IT 75-16-1, Methylmagnesium bromide
RL: RCT (Reactant)
(Grignard reaction of, with alanine thioester deriv., in prepn. of azasteroidal 5.alpha.-reductase inhibitors)
IT 407-25-0, Trifluoroacetic anhydride
RL: RCT (Reactant)
(acylation by, of oxazolone deriv., in prepn. of azasteroidal 5.alpha.-reductase inhibitors)
IT 2491-18-1, L-Methionine methyl ester hydrochloride 5813-64-9, Neopentylamine 13404-22-3, L-Alanine tert-butyl ester hydrochloride 103335-49-5 103335-50-8 156990-65-7
RL: RCT (Reactant)
(amidation of, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)
IT 302-72-7, D,L-Alanine 516-06-3, D,L-Valine
RL: RCT (Reactant)
(benzoylation of, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)
IT 433-27-2, Trifluoroacetaldehyde ethyl hemiacetal
RL: RCT (Reactant)

(condensation of, with nitropropane, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)

IT 79-46-9, 2-Nitropropane
RL: RCT (Reactant)
(condensation of, with trifluoroacetaldehyde Et hemiacetal, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)

IT 328-39-2, D,L-Leucine
RL: PROC (Process)
(conversion of, to (acetylamino)methylhexanone, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)

IT 17463-43-3, D,L-Trifluoroalanine
RL: PROC (Process)
(conversion of, to (acetylamino)trifluorobutanone, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)

IT 20859-02-3, L-tert-Leucine
RL: RCT (Reactant)
(ethoxycarbonylation of, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)

IT 9081-34-9, Testosterone 5.alpha.-reductase
RL: RCT (Reactant)
(inhibitors of, azaandrostanone derivs. as)

IT 1205-02-3P 15734-82-4P 51127-13-0P 123206-07-5P 123206-10-0P
155651-62-0P 156990-36-2P, (S)-2-Aminoheptan-3-one hydrochloride
156990-37-3P, 3-Methyl-3-nitro-1,1,1-trifluorobutan-2-ol
156990-38-4P, N-(Ethoxycarbonyl)-3-amino-4,4,-dimethylpentan-2-one
156990-39-5P, (R)-3-Amino-4,4-dimethylpentan-2-one hydrobromide
156990-46-4P 156990-47-5P 156990-48-6P 156990-49-7P
156990-50-0P 156990-51-1P 156990-52-2P 156990-53-3P
156990-54-4P 156990-55-5P 156990-56-6P 156990-57-7P
156990-58-8P 156990-59-9P 156990-60-2P 156990-61-3P
156990-62-4P 156990-66-8P, (S)-3-Amino-4,4-dimethylpentan-2-one hydrobromide 157085-86-4P 157085-87-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, as intermediate for testosterone 5.alpha.-reductase inhibitor)

IT 155651-61-9P 156990-08-8P 156990-09-9P 156990-10-2P
156990-11-3P 156990-12-4P 156990-13-5P 156990-14-6P
156990-15-7P 156990-16-8P 156990-17-9P 156990-18-0P
156990-19-1P 156990-20-4P 156990-21-5P 156990-22-6P
156990-23-7P 156990-24-8P 156990-25-9P 156990-26-0P
156990-27-1P 156990-28-2P 156990-29-3P 156990-30-6P
156990-31-7P 156990-32-8P 156990-33-9P 156990-34-0P
156990-35-1P 156990-40-8P 156990-41-9P 156990-42-0P
156990-43-1P 156990-44-2P 156990-45-3P 157085-66-0P
157085-67-1P 157085-68-2P 157085-69-3P 157085-70-6P
157085-71-7P 157085-72-8P 157085-73-9P 157085-74-0P
157085-75-1P 157085-76-2P 157085-77-3P 157085-78-4P
157085-79-5P 157085-80-8P 157085-81-9P 157085-82-0P
157085-83-1P 157085-84-2P 157085-85-3P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of, as testosterone 5.alpha.-reductase inhibitor)

IT 15761-38-3, BOC-Ala-OH

RL: RCT (Reactant)
(reaction of, with butyllithium, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)

IT 109-72-8, n-Butyllithium, reactions
RL: RCT (Reactant)
(reaction of, with protected alanine, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)

IT 917-54-4, Methyllithium
RL: RCT (Reactant)
(reaction of, with tert-butylleucine deriv., in prepn. of azasteroidal 5.alpha.-reductase inhibitors)

IT 541-41-3, Ethyl chloroformate
RL: RCT (Reactant)
(reaction of, with tert-butylleucine, in prepn. of azasteroidal 5.alpha.-reductase inhibitors)

L7 ANSWER 2 OF 7 MARPAT COPYRIGHT 1995 ACS
(ALL HITs ARE ITERATION INCOMPLETES)
AN 121:109397 MARPAT
TI Preparation of ester derivatives of 4-azasteroids as steroid 5.alpha.-reductase inhibitors.
IN Witzel, Bruce E.; Rasmusson, Gary H.; Tolman, Richard L.; Yang, Shu Shu
PA Merck and Co., Inc., USA
SO PCT Int. Appl., 66 pp.
CODEN: PIXXD2
PI WO 9323041 A1 931125
DS W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KR, KZ, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AI WO 93-US4771 930519
PRAI US 92-886022 920520
DT Patent
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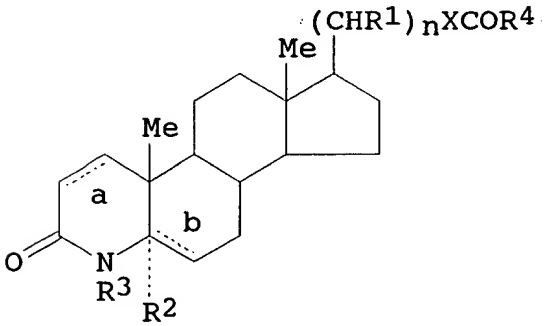

I

AB Title compds. [I; a, b = single bonds, R2 = H; or a = single bond, b = double bond, and R2 = null; R1 = H, aryl, alkyl, aralkyl; R3 = H,

Me, Et, OH, NH2, SMe; n = 0-10; X = O, S; R4 = (substituted) alkyl, aryl, heterocyclyl, cycloalkyl, amino, OH, etc.] were prepd. as inhibitors of 5.alpha.-reductase and isoenzymes thereof. The compds. are useful for the treatment of hyperandrogenic disease conditions and diseases of the skin and scalp (no data). Thus, 20-hydroxy-4-methyl-5.alpha.-4-azapregnan-3-one, 11-ethylthioundecanoic acid, DMAP, and DCC were stirred in CH2Cl2 at room temp. to give 20-[11-(ethylthio)undecanoyloxy]-4-methyl-5.alpha.-4-azapregnan-3-one.

IC ICM A61K031-435
ICS C07D221-02

CC 32-4 (Steroids)
Section cross-reference(s): 1

ST azasteroid ester prepn steroid reductase inhibitor

IT Hirsutism
(female, treatment of, azasteroid esters for)

IT Acne
(treatment of, azasteroid esters for)

IT Prostate gland
(disease, benign hyperplasia, treatment of, azasteroid esters for)

IT Prostate gland
(disease, prostatitis, treatment of, azasteroid esters for)

IT Alopecia
(male pattern, treatment of, azasteroid esters for)

IT Prostate gland
(neoplasm, carcinoma, treatment of, azasteroid esters for)

IT 9081-34-9, 5.alpha.-Steroid reductase
RL: USES (Uses)
(inhibitors, azasteroid esters as)

IT 104214-41-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 156804-81-8P 156804-82-9P 156804-83-0P 156804-84-1P
156804-85-2P 156804-86-3P 156804-87-4P 156804-88-5P
156804-89-6P 156804-90-9P 156804-91-0P 156804-92-1P
156804-93-2P 156804-94-3P 156804-95-4P 156804-96-5P
156804-97-6P 156804-98-7P 156804-99-8P 156805-00-4P
156805-01-5P 156805-02-6P 156805-03-7P 156805-04-8P
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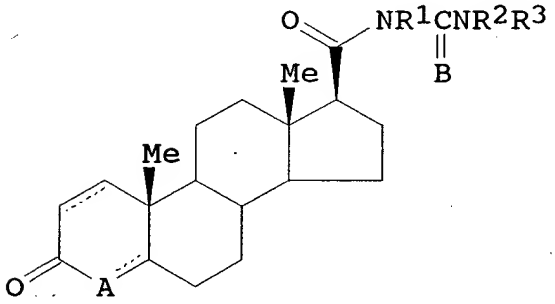
156805-13-9P 156805-14-0P 156805-15-1P 156805-16-2P
156805-17-3P 156804-18-4P 156805-19-5P 156805-20-8P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of, as steroid 5.alpha.-reductase inhibitor)

IT 624-83-9, Methyl isocyanate 627-03-2, Ethoxyacetic acid
1609-86-5, tert-Butyl isocyanate 3173-56-6, Benzyl isocyanate
3282-30-2, Trimethylacetyl chloride 38460-95-6, 10-Undecenoyl chloride 76318-67-7 86284-02-8 104319-27-9 114019-70-4, 11-Ethylthioundecanoic acid 144879-14-1 156804-93-2
156805-21-9 156924-96-8
RL: RCT (Reactant)

(reaction of, in prepn. of steroid 5.alpha.-reductase inhibitor)

L7 ANSWER 3 OF 7 MARPAT COPYRIGHT 1995 ACS
AN 121:83749 MARPAT
TI Preparation of steroids with fluorinated acylureidic side chains as testosterone 5.alpha.-reductase inhibitors
IN Panzeri, Achille; Nesi, Marcella; Di, Salle Enrico
PA Farmitalia Carlo Erba S.R.L., Italy
SO PCT Int. Appl., 44 pp.
CODEN: PIXXD2
PI WO 9403474 A1 940217
DS W: JP
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI WO 93-EP2035 930729
PRAI GB 92-16280 920731
DT Patent
LA English
GI



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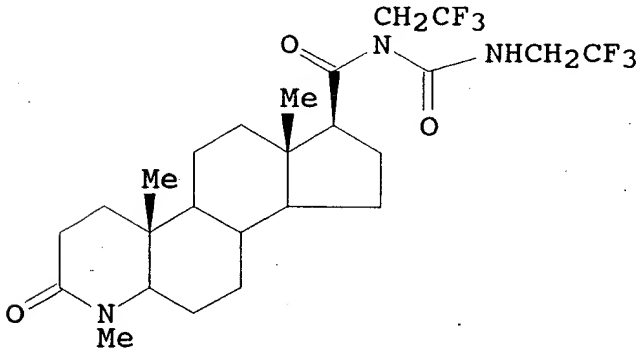

II

AB 5.alpha.-Reductase inhibitors (I; dotted line = optional double bond; A = CH, NR; R = H, C1-C4 alkyl; B = O,S; R1-R3 = H, C1-C6 alkyl group or an aryl group wherein, optionally, one or more hydrogen atoms are substituted by one or more fluorine atoms), with provisos, were prepd. The compds. of the invention are therapeutically useful in, e.g., benign prostatic hyperplasia,

prostatic and breast cancers, seborrhea, female hirsutism and male pattern baldness (no data). Thus, 1,3-di(2,2,2-trifluoroethyl)urea was refluxed with CCl4, Et3N, and Ph3P in CH2Cl2 for 2 h; 4-methyl-3-oxo-4-aza-androstane-17.beta.-carboxylic acid was added and the mixt. was stirred overnight to give title compd. II. Tablets were prepd. contg. II.

IC ICM C07J073-00
ICS C07J041-00; A61K031-56; A61K031-58

CC 32-4 (Steroids)
Section cross-reference(s): 1

ST azaoxoandrostanecarbonylurea fluorinated prepn testosterone reductase inhibitor; oxoandrostenecarbonylurea fluorinated prepn testosterone reductase inhibitor

IT Steroids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, with fluorinated carbonylurea side chains, as testosterone 5.alpha.-reductase inhibitors)

IT 9081-34-9, Testosterone 5.alpha.-reductase
RL: USES (Uses)
(inhibitors, steroids with fluorinated carbonylurea side chains as)

IT 406-11-1P, 1,3-Bis(2,2,2-trifluoroethyl)urea 156137-50-7P
156137-51-8P 156137-52-9P, 1,1-Diethyl-3-(2,2,2-trifluoroethyl)urea
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for testosterone 5.alpha.-reductase inhibitor)

IT 156137-35-8P 156137-36-9P 156137-37-0P 156137-38-1P
156137-39-2P 156137-40-5P 156137-41-6P 156137-42-7P
156137-43-8P 156137-44-9P 156137-45-0P 156137-46-1P
156137-47-2P 156137-48-3P 156137-49-4P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of, as testosterone 5.alpha.-reductase inhibitor)

IT 88-10-8, N,N-Diethylcarbamoyl chloride 109-90-0, Ethyl isocyanate 373-88-6, 2,2,2-Trifluoroethylamine hydrochloride 753-90-2, 2,2,2-Trifluoroethylamine 32315-10-9, Triphosgene 76763-16-1 76763-18-3 155651-52-8 156137-47-2
RL: RCT (Reactant)
(reaction of, in prepn. of testosterone 5.alpha.-reductase inhibitor)

L7 ANSWER 4 OF 7 MARPAT COPYRIGHT 1995 ACS
AN 121:57781 MARPAT
TI Fluorinated 17.beta.-substituted 4-aza-5.alpha.-androstan-3-one derivatives useful as testosterone 5.alpha.-reductase inhibitors, and their preparation
IN Panzeri, Achille; Nesi, Marcella; Di Salle, Enrico
PA Farmitalia Carlo Erba S.R.L., Italy
SO PCT Int. Appl., 70 pp.
CODEN: PIXXD2
PI WO 9403475 A1 940217
DS W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP,

KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 93-EP2037 930729
PRAI GB 92-16284 920731
DT Patent
LA English
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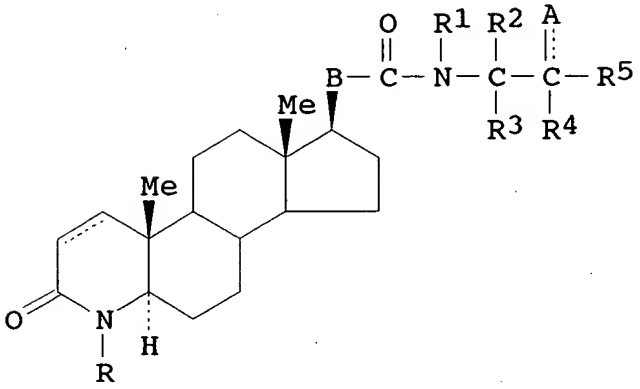

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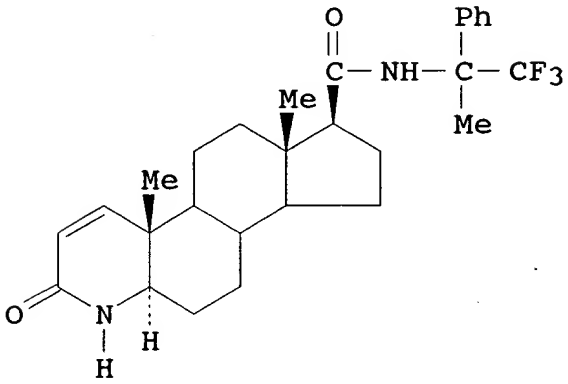


II

AB Title steroids I [B = bond, straight or branched C1-C6 alkylene; R = H, C1-C4 (fluoro)alkyl; R1 = H, C1-C6 (fluoro)alkyl, benzyl; R2 = (a) H, F, C1-C6 (fluoro)alkyl, C5-C7 cycloalkyl, C6-C9 cycloalkylalkyl; or (b) (un)substituted aryl or C7-C10 arylalkyl; R3 = (a) H, F, C1-C4 (fluoro)alkyl; or (b) (un)substituted aryl or C7-C10 arylalkyl; R4 = H, F, or is absent when A is bound by double bond; R5 = H, F, C1-C6 (fluoro)alkyl; A = H, F, CR6R7R8, :CR6R7; R6, R7, R8 = H, F, C1-C6 (fluoro)alkyl; with the proviso that .gtoreq. 1 of groups R-R5 or A contains .gtoreq. 1 F atom], including 44 specifically named compds., are claimed, and several example prepns. are given. For example, S-(2-pyridyl) 3-oxo-4-aza-5.alpha.-andros-1-ene-17.beta.-carbothioate was treated with MeI in CH2Cl2 and then

with (.+-.)-PhC(Me)(CF3)NH2 in DMF, and the mixt. was heated at 100.degree. for 8 h to give title compd. II. At 3 mg/kg/day orally, II gave 54% inhibition of testosterone-induced prostatic hypertrophy in castrated rats. Three std. pharmaceutical formulations are described.

IC ICM C07J073-00
ICS A61K031-58

CC 32-4 (Steroids)
Section cross-reference(s): 1, 2

ST fluorinated azaandrostanone prepn testosterone reductase inhibitor; androstanone aza fluorinated prepn antiandrogen

IT Hirsutism
(female, treatment of, fluorinated azaandrostanone derivs. for)

IT Neoplasm inhibitors
(fluorinated azaandrostanone derivs.)

IT Acne
Seborrhea
(treatment of, fluorinated azaandrostanone derivs. for)

IT Steroids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(4-aza-, oxo, fluorinated, prepn. of, as testosterone 5.alpha.-reductase inhibitors)

IT Androgens
RL: RCT (Reactant)
(antiandrogens, fluorinated azaandrostanone derivs.)

IT Prostate gland
(disease, benign hyperplasia, treatment of, fluorinated azaandrostanone derivs. for)

IT Alopecia
(male pattern, treatment of, fluorinated azaandrostanone derivs. for)

IT Mammary gland
Prostate gland
(neoplasm, treatment of, fluorinated azaandrostanone derivs. for)

IT 155651-61-9
RL: RCT (Reactant)
(Wittig reaction of, in prepn. of antiandrogens)

IT 2065-66-9, Methyltriphenylphosphonium iodide
RL: RCT (Reactant)
(Wittig reaction of, with azasteroidal ketone, in prepn. of antiandrogens)

IT 434-45-7, Trifluoroacetophenone
RL: RCT (Reactant)
(Wittig-type reaction of, with (carbethoxy)triphenylphosphineimine, in prepn. of antiandrogens)

IT 17437-51-3, N-(Ethoxycarbonyl)triphenylphosphinimine
RL: RCT (Reactant)
(Wittig-type reaction of, with trifluoroacetophenone, in prepn. of antiandrogens)

IT 103335-49-5 104214-40-6
RL: RCT (Reactant)
(amidation of, with fluorinated amines, in prepn. of antiandrogens)

IT 373-88-6, 2,2,2-Trifluoroethylamine hydrochloride 753-90-2, 2,2,2-Trifluoroethylamine 155651-15-3
RL: RCT (Reactant)
(amidation of, with steroidal thioester, in prepn. of antiandrogens)

IT 155651-27-7
RL: RCT (Reactant)
(hydrogenation of, in prepn. of antiandrogens)

IT 9081-34-9, Testosterone 5.alpha.-reductase
RL: RCT (Reactant)
(inhibitors of, prepn. of fluorinated azaandrostanone derivs. as)

IT 155651-16-4P, (.+-.)-1-Trifluoromethyl-1-phenylethylamine 155651-64-2P, (RS)-1-Trifluoromethyl-1-phenylethylamine hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and amidation of, with steroidal thioester, in prepn. of antiandrogens)

IT 155651-60-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of, in prepn. of antiandrogens)

IT 63116-59-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with methylmagnesium iodide, in prepn. of antiandrogens)

IT 155651-63-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. of, in prepn. of antiandrogens)

IT 155651-17-5P 155651-18-6P 155651-19-7P 155651-20-0P
155651-21-1P 155651-22-2P 155651-23-3P 155651-24-4P
155651-25-5P 155651-26-6P 155651-27-7P 155651-28-8P
155651-29-9P 155651-30-2P 155651-31-3P 155651-32-4P
155651-33-5P 155651-34-6P 155651-35-7P 155651-36-8P
155651-37-9P 155651-38-0P 155651-39-1P 155651-40-4P 155651-41-5P 155651-42-6P 155651-43-7P 155651-44-8P 155651-45-9P
155651-46-0P 155651-47-1P 155651-48-2P 155651-49-3P
155651-50-6P 155651-51-7P 155651-52-8P 155651-53-9P
155651-54-0P 155651-55-1P 155651-56-2P 155651-57-3P
155651-58-4P 155651-59-5P 155850-26-3P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of, as testosterone 5.alpha.-reductase inhibitor)

IT 917-64-6, Methylmagnesium iodide
RL: RCT (Reactant)
(reaction of, with trifluorophenylethanimine deriv., in prepn. of antiandrogens)

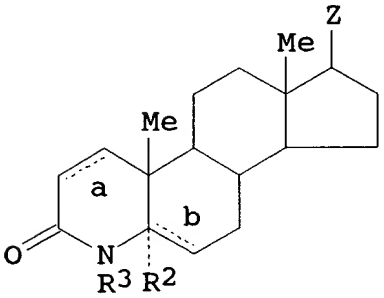
IT 155651-62-0
RL: RCT (Reactant)
(thioesterification and redn. of, in prepn. of antiandrogens)

L7 ANSWER 5 OF 7 MARPAT COPYRIGHT 1995 ACS
(ALL HITs ARE ITERATION INCOMPLETES)
AN 120:245602 MARPAT
TI Preparation of 17-ethers and thioethers of 4-aza-steroids as steroid

reductase inhibitors

IN Witzel, Bruce E.; Tolman, Richard L.; Rasmusson, Gary H.; Bakshi, Raman K.; Yang, Shu Shu
PA Merck and Co., Inc., USA

SO PCT Int. Appl., 68 pp.
CODEN: PIXXD2
PI WO 9323040 A1 931125
DS W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KR, KZ, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AI WO 93-US4746 930519
PRAI US 92-886031 920520
DT Patent
LA English
GI



I

AB Title compds. [I; a, b both = single bonds, and R2 = H; or a = double bond, b = single bond, and R2 = H; or a = single bond, b = double bond, and R2 = null; R1 = H, aryl, (aryl)alkyl; R3 = H, Me, Et, OH, NH2, SMe; R4 = (substituted) alkyl, aryl, heterocyclyl; Z = XR4, (CHR1)nXR4; X = O, S, SO, SO2], were prepd. as inhibitors of steroid 5.alpha.-reductase enzymes 1 and 2 (no data). The compds. are useful for the treatment of hyperandrogenic disease conditions and diseases of the skin and scalp. Thus, 17-hydroxymethyl-4-methyl-5.alpha.-4-azaandrostan-3-one and diphenyldiazomethane in CH2Cl2 were treated dropwise with BF3.Et2O to give 17-diphenylmethoxymethyl-4-methyl-5.alpha.-4-azaandrostan-3-one.

IC ICM A61K031-435
ICS C07D221-02
CC 32-4 (Steroids)
Section cross-reference(s): 1
ST azasteroid ether prepn reductase inhibitor; testosterone reductase inhibitor azasteroid ether; prostatitis treatment azasteroid ether; hyperplasia treatment azasteroid ether; hirsutism treatment azasteroid ether; carcinoma prostatic treatment azasteroid ether
IT Hirsutism
(female, treatment of, azasteroid ethers for)
IT Acne

(treatment of, azasteroid ethers for)

IT Steroids, preparation
(4-aza-, 17-(thio)ethers, prepn. of, as steroid reductase inhibitors)

IT Prostate gland
(disease, benign hyperplasia, treatment of, azasteroid ethers for)

IT Prostate gland
(disease, prostatitis, treatment of, azasteroid ethers for)

IT Alopecia
(male pattern, treatment of, azasteroid ethers for)

IT Prostate gland
(neoplasm, carcinoma, treatment of, azasteroid ethers for)

IT 9081-34-9, 5.alpha.-Reductase
(inhibitors, azasteroid ethers as)

IT 153946-18-0P 153946-19-1P 153946-20-4P 153946-21-5P
153946-22-6P 153946-23-7P 153946-24-8P 153946-25-9P
153946-27-1P
(prepn. of, as intermediate for steroid 5.alpha.-reductase inhibitor)

IT 153945-26-7P 153945-27-8P 153945-28-9P 153945-29-0P
153945-30-3P 153945-31-4P 153945-32-5P 153945-33-6P
153945-34-7P 153945-35-8P 153945-36-9P 153945-37-0P
153945-38-1P 153945-39-2P 153945-40-5P 153945-41-6P
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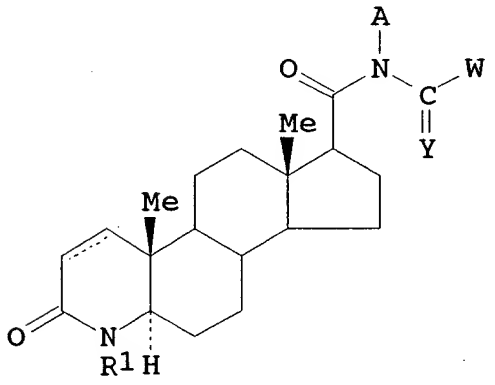
153946-02-2P 153946-03-3P 153946-04-4P 153946-05-5P
153946-06-6P 153946-07-7P 153946-08-8P 153946-09-9P
153946-10-2P 153946-11-3P 153946-12-4P 153946-13-5P
153946-14-6P 153946-15-7P 153946-16-8P 153946-17-9P
(prepn. of, as steroid 5.alpha.-reductase inhibitor)

IT 70-34-8, 2,4-Dinitrofluorobenzene 75-12-7, Formamide, reactions
92-69-3, 4-Hydroxybiphenyl 99-92-3, 4-Aminoacetophenone
102-49-8, 3,4-Dichlorobenzylamine 324-74-3, 4-Fluorobiphenyl
334-88-3, Diazomethane 350-46-9 352-32-9, 4-Fluorotoluene
352-33-0, 4-Fluorochlorobenzene 372-47-4, 3-Fluoropyridine
405-99-2, 4-Fluorostyrene 460-00-4, 4-Fluorobromobenzene
623-73-4, Ethyl diazoacetate 638-45-9, Hexyl iodide 769-92-6
811-51-8, Sodium thioethoxide 883-40-9, Diphenyldiazomethane
933-40-4, 1,1-Dimethoxycyclohexane 1194-02-1 4377-33-7,

2-Picolyl chloride 20607-43-6 52267-51-3, Benzyl diazoacetate 86283-92-3 86284-02-8 104214-41-7 104319-27-9 153946-26-0 153946-28-2 153946-29-3 154006-53-8
(reaction of, in prepn. of steroid 5.alpha.-reductase inhibitor)

L7 ANSWER 6 OF 7 MARPAT COPYRIGHT 1995 ACS
AN 115:256467 MARPAT
TI Preparation of 17.beta.-carbamoyl-4-azaandrostan-3-ones as testosterone 5.alpha.-reductase inhibitors
IN Panzeri, Achille; Di Salle, Enrico; Nesi, Marcella
PA Farmitalia Carlo Erba S.r.l., Italy
SO PCT Int. Appl., 87 pp.
CODEN: PIXXD2
PI WO 9112261 A1 910822
DS W: AU, CA, FI, HU, JP, KR, NO, SU
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE
AI WO 91-EP228 910206
PRAI GB 90-2922 900209
DT Patent
LA English
GI



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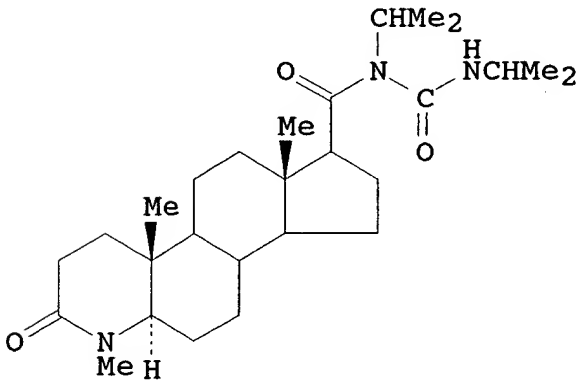

II

AB Title compds. [I; R1 = H, alkyl, arylalkyl, aroyl; Y = O, S; W = NR2R3; R2, R3 = H, (substituted) (cyclo)alkyl, cycloalkylalkyl, aryl; A = H, (substituted) (cyclo)alkyl, cycloalkylalkyl; dotted line indicates optional bond], were prepd. Thus, 4-methyl-4-aza-5.alpha.-androstan-3-one-17.beta.-carboxylic acid (prepn. from 4-methyl-4-aza-5.alpha.-androstane-3,17-dione given) in CH2Cl2 was stirred overnight with N,N'-diisopropylcarbodiimide to give title compd. II. The latter at 10 mg/kg orally daily in rats gave 55% inhibition of testosterone propionate-stimulated prostate growth. Oral dosage forms were prepd. contg. II.

IC ICM C07J073-00
ICS A61K031-56; A61K031-58

CC 32-4 (Steroids)
Section cross-reference(s): 1, 63

ST carbamoylazaandrostanone prepn testosterone reductase inhibitor; azaandrostenone carbamoyl testosterone reductase inhibitor

IT 109-90-0, Ethyl isocyanate
(acylation by, (aminopropylcarbamyl)androstenone deriv.)

IT 109-55-7, 3-Dimethylaminopropylamine
(amidation by, of azaandrostanecarboxylate)

IT 693-13-0, N,N'-Diisopropylcarbodiimide
(condensation of, with azaandrastanonecarboxylic acid)

IT 96692-02-3 104239-97-6
(condensation of, with diisopropylcarbodiimide, in prepn. of testosterone 5.alpha.-reductase inhibitor)

IT 86284-03-9
(conversion of, to cyanohydrin, in prepn. of testosterone 5.alpha.-reductase inhibitor)

IT 9036-43-5, Testosterone 5.alpha.-reductase 37255-34-8, Testosterone 5.alpha.-reductase
(inhibitors, carbamoylazaandrastanones)

IT 76763-18-3P
(prepn. and condensation of, with dimethylthioformamide, in prepn. of testosterone 5.alpha.-reductase inhibitor)

IT 76763-16-1P 103335-55-3P 137099-81-1P 137099-82-2P
137099-83-3P 137099-84-4P 137099-85-5P 137099-86-6P
137099-87-7P 137099-88-8P 137099-90-2P 137099-91-3P
(prepn. of, as intermediate for testosterone 5.alpha.-reductase inhibitor)

IT 137099-09-3P 137099-10-6P 137099-11-7P 137099-12-8P
137099-13-9P 137099-14-0P 137099-15-1P 137099-16-2P
137099-17-3P 137099-18-4P 137099-19-5P 137099-20-8P
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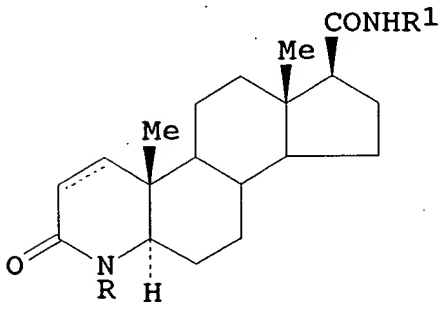
137121-97-2P 137121-98-3P 137121-99-4P 137122-00-0P
137127-06-1P 137127-07-2P 137127-08-3P 137127-09-4P
137127-10-7P 137127-11-8P 137127-12-9P 137127-13-0P
(prepn. of, as testosterone 5.alpha.-reductase inhibitor)

IT 103335-49-5 104214-40-6 137099-89-9 137146-68-0
(reaction of, in prepn. of testosterone 5.alpha.-reductase inhibitor)

IT 758-16-7, Dimethylthioformamide
(reaction of, with azaandrostanecarbonyl chloride deriv.)

L7 ANSWER 7 OF 7 MARPAT COPYRIGHT 1995 ACS
AN 109:129456 MARPAT
TI Preparation of antiandrogenic, oxidized analogs of 17.beta.-(N-monosubstituted carbamoyl)-4-aza-5.alpha.-androstan-3-ones
IN Carlin, Josephine R.; Rasmusson, Gary H.; Vandenheuvel, W. J. A.
PA Merck and Co., Inc., USA
SO Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
PI EP 271220 A1 880615
DS R: AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, NL, SE
AI EP 87-309951 871111
PRAI US 86-932550 861120
DT Patent
LA English
GI



I

AB Title compds. I (R = H, Me, Et; R1 = C1-12 straight or branched alkyl wherein 1 H atom is substituted by OH, CO2H, or C1-4 alkyl ester; dotted line = optional double bond), some of which are oxidn. metabolites of I (R = H, R1 = CMe3, .DELTA.1 present) (II), are prepd. for use as testosterone 5.alpha.-reductase inhibitors (no data). Coupling of 3-oxo-4-aza-5.alpha.-androst-1-ene-17.beta.-

carboxylic acid with H2NCMe2CH2OH using DCC and 1-hydroxybenzotriazole in CH2Cl2 gave I (R = H, R1 = CMe2CH2OH, .DELTA.1 present), a major plasma metabolite of II.

IC ICM C07J073-00
ICS A61K031-435; A61K031-58

CC 32-4 (Steroids)
Section cross-reference(s): 2

ST carbamoylazaandrostanone prepn antiandrogen; azaandrostanone carbamoyl prepn antiandrogen; androstanone carbamoylaza prepn antiandrogen

IT Androgens
(inhibitors, carbamoylazaandrostanones)

IT Hirsutism
Seborrhea
(treatment of, carbamoylazaandrostanones for)

IT Steroids, preparation
(4-aza-, prepn. of carbamoylazaandrostanones, as testosterone reductase inhibitors)

IT Prostate gland
(disease, benign hyperplasia, treatment of, carbamoylazaandrostanones for)

IT Acne
(vulgaris, treatment of, carbamoylazaandrostanones for)

IT 76763-16-1 103335-50-8 104239-97-6
(amidation of, with alkylamine derivs.)

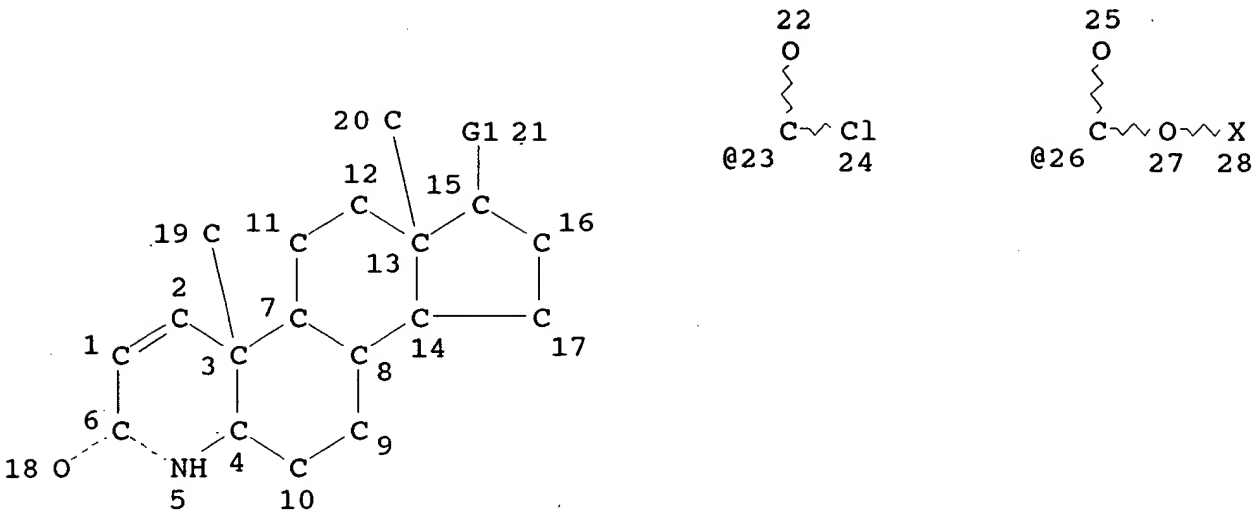
IT 124-68-5, 2-Amino-2-methyl-1-propanol 141-43-5, reactions 616-34-2, Methyl glycinate
(amidation of, with androstanonecarboxylic acid derivs.)

IT 98319-26-7
(antiandrogenic oxidized metabolites of)

IT 9036-43-5, Testosterone 5.alpha.-reductase
(inhibitors of, carbamoylazaandrostanones as)

IT 104214-50-8P 104214-51-9P 104214-52-0P 116285-36-0P 116285-37-1P 116285-38-2P 116285-39-3P 116285-40-6P 116285-41-7P 116285-42-8P
(prepn. of, as antiandrogen)

=> d que stat; fil reg
L5 STR



VAR G1=23/26
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:
ECLEVEL IS LIM ON ALL NODES
ALL RING(S) ARE ISOLATED

L8 0 SEA FILE=MARPATPREV SSS FUL L5 (MODIFIED ATTRIBUTES)

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.04

FILE 'REGISTRY' ENTERED AT 12:51:59 ON 03 NOV 95

STRUCTURE FILE UPDATES: 27 OCT 95 HIGHEST RN 169435-71-6
DICTIONARY FILE UPDATES: 2 Nov 95 HIGHEST RN 169435-71-6

TSCA INFORMATION NOW CURRENT THROUGH JUNE 1995

Please note that search-term pricing does apply when conducting SmartSELECT searches.

claim 1

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=> s ?"phenylcarbamoyl-4-aza-5.alpha.-androst"?/cns
          1918 ?"PHENYLCARBAMOYL"/CNS
       4603330 "4"/CNS
         12443 "AZA"/CNS
         42544 "5.ALPHA."/CNS
         49982 "ANDROST"?/CNS
L9           0 ?"PHENYLCARBAMOYL-4-AZA-5.ALPHA.-ANDROST"?/CNS
                 ((?"PHENYLCARBAMOYL"(W)"4"(W)"AZA"(W)"5.ALPHA."(W)"ANDRO
                 ST"?)/CNS)

=> fil ca; s 17(w)(b or beta)(l)androst
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FILE COVERS 1967 - 28 Oct 1995 (951028/ED)  VOL 123 ISS 18

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  SmartSELECT searches with large numbers of terms.

  CAS Roles are here!  Roles are available for records from July 1994
  to date.


        279254 17
        637526 B
        616392 BETA
          2577 ANDROST
L10       1044 17(W)(B OR BETA)(L)ANDROST

=> s l10(l)(phenylcarbamoyl? or phenyl carbamoyl?)
          1234 PHENYLCARBAMOYL?
        127244 PHENYL
         17478 CARBAMOYL?
           147 PHENYL CARBAMOYL?
                 (PHENYL(W)CARBAMOYL?)
L11          5 L10(L)(PHENYLCARBAMOYL? OR PHENYL CARBAMOYL?)

=> fil caplus; s l11
FILE 'CAPLUS' ENTERED AT 12:54:18 ON 03 NOV 95
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        282534 17
        645567 B
        622741 BETA
          2595 ANDROST
          1236 PHENYLCARBAMOYL?
        128092 PHENYL
         17591 CARBAMOYL?
           150 PHENYL CARBAMOYL?
                 (PHENYL(W)CARBAMOYL?)
L12           5 L10(L)(PHENYLCARBAMOYL? OR PHENYL CARBAMOYL?)

=> dup rem l11,l12
FILE 'CA' ENTERED AT 12:54:28 ON 03 NOV 95
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PROCESSING COMPLETED FOR L11
PROCESSING COMPLETED FOR L12
L13           5 DUP REM L11 L12 (5 DUPLICATES REMOVED)

=> d 1-5 .bevstr1

L13  ANSWER 1 OF 5  CA  COPYRIGHT 1995 ACS              DUPLICATE 1
AN   123:56393  CA
TI   Androstenone derivative
IN   Batchelor, Kenneth William; Frye, Stephen Vernon
PA   Glaxo Inc., USA
SO   PCT Int. Appl., 23 pp.
     CODEN: PIXXD2
PI   WO 9507927 A1  950323
DS   W:  AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI,
         GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG,
         MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA,
         US, UZ
     RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR,
         IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AI   WO 94-US10530  940916
PRAI US 93-123280  930917
DT   Patent
LA   English
AB   The present invention relates to 17.beta
     .-N-[2,5-bis(trifluoromethyl)phenyl]carbamoyl
     -4-aza-5.alpha.-androst-1-en-3-one (I), solvates thereof,
     its prepn., intermediates used in its prepn., pharmaceutical
     formulations thereof and its use in the treatment of
     androgen-responsive and -mediated diseases.  Thus,
     3-oxo-4-androstene-17.beta.-carboxylic acid was
     carbamoylated, subjected to oxidative cleavage of the A-ring,
```

recyclized with NH3, and reduced to give I, which is a strong selective inhibitor of testosterone 5.alpha.-reductase.

IT 164656-23-9P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(bis(trifluoromethyl)phenylcarbamoylazaandrostenone as testosterone reductase inhibitor)

IT 9081-34-9, Testosterone 5.alpha.-reductase
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(bis(trifluoromethyl)phenylcarbamoylazaandrostenone as testosterone reductase inhibitor)

IT 302-97-6, 3-Oxo-4-androstene-17.beta.-carboxylic acid 328-93-8, 2,5-Bis(trifluoromethyl)aniline
RL: RCT (Reactant)
(bis(trifluoromethyl)phenylcarbamoylazaandrostenone as testosterone reductase inhibitor)

IT 164656-19-3P 164656-20-6P 164656-21-7P 164656-22-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(bis(trifluoromethyl)phenylcarbamoylazaandrostenone as testosterone reductase inhibitor)

L13 ANSWER 2 OF 5 CA COPYRIGHT 1995 ACS DUPLICATE 2
AN 97:145135 CA
TI 14.beta.-Hydroxy steroids
PA Akademie der Wissenschaften der DDR, Zentralinstitut fuer Mikrobiologie und Experimentelle Therapie, Ger. Dem. Rep.
SO Ger. (East), 13 pp.
CODEN: GEXXA8
PI DD 151946 Z 811111
AI DD 80-222404 800704
DT Patent
LA German
AB 14.beta.-Hydroxy steroids were prepd. from **17.beta**.-carbamoyloxy-14-unsatd. steroids by successive epoxidn. and redn. Thus, epoxidn. of **17.beta.-(phenylcarbamoyloxy)**androsta-4,14-dien-3-one by 3-chloroperbenzoic acid gave 14.beta.,15.beta.-epoxy-**17.beta.-(phenylcarbamoyloxy)androst**-4-en-3-one, which was reduced by LiAlH4 in THF to give **androst**-4-ene-3.beta.,14.beta.,**17.beta**.-triol. Jones oxidn. of the latter gave 14.beta.-hydroxyandrost-4-ene-3,17-dione.

IT Epoxidation
(of carbamoyloxy unsatd. steroids)

IT 19-Norsteroids
(prepn. of, of hydroxy deriv., by epoxidn.-redn. of unsatd. carbamoyloxy deriv.)

IT Steroids, preparation
(prepn. of, of hydroxy steroids, via epoxidn.-redn. of unsatd. carbamoyloxy steroids)

IT 1035-77-4 35644-61-2 60752-62-7 82792-30-1

(addn. reaction of, with Ph isocyanate)
IT 3019-71-4
(addn. reaction of, with trihydroxyandrostane)
IT 103-71-9, reactions
(addn. reactions of, with hydroxy steroids)
IT 24357-35-5 82792-39-0
(carbamoylation of)
IT 82792-31-2P
(prepn. and deacetylation of)
IT 81164-67-2P 82792-26-5P 82792-33-4P 82792-36-7P
(prepn. and epoxidn. of)
IT 82792-28-7P
(prepn. and oxidn. and acetylation of)
IT 82792-32-3P 82792-35-6P 82792-38-9P
(prepn. and oxidn. of)
IT 81203-66-9P 82792-27-6P 82792-34-5P 82792-37-8P 82863-09-0P
(prepn. and redn. of)
IT 2919-59-7P 38676-87-8P 60183-64-4P 82792-29-8P 82837-90-9P
82837-91-0P 82837-92-1P
(prepn. of)

L13 ANSWER 3 OF 5 CA COPYRIGHT 1995 ACS DUPLICATE 3
AN 77:140411 CA
TI Steroid oxime carbamic acid esters
IN Ponsold, Kurt; Wagner, Horst
SO Ger. (East), 2 pp.
CODEN: GEXXA8
PI DD 89613 720505
AI DD 69-137449 690124
DT Patent
LA German
AB Steroid oximes reacted with RNCO (R = alkyl, aryl) to give the cor-responding O-carbamoyl steroid oximes. Thus, **androst-4-en-17.beta.-ol-3-one** oxime propionate was treated with PhNCO to give O-(**phenylcarbamoyl**) **androst-4-en-17.beta.-ol-3-one** oxime propio-nate. Similarly, 3 estratriene oxime derivs. (I, R, R2, R3 = H, OH, MeO: R1 = Et, Ph) were prepd.
IT Steroids, preparation
(oxo, O-carbamoyloximes)
IT 37926-71-9P 37926-72-0P 37926-73-1P 37926-74-2P
(prepn. of)

L13 ANSWER 4 OF 5 CA COPYRIGHT 1995 ACS DUPLICATE 4
AN 75:77127 CA
TI Steroids. 28. Preparation of steroid hormone analogs from 2,3.beta.-imino-5.alpha.-androstan-17.beta.-ol and 2.beta.-amino-3.alpha.-chloro-5.alpha.-androstan-17.beta.-ol
AU Ponsold, Kurt; Preibsch, Wolfgang
CS Zentralinst. Mikrobiol. Exp. Ther., Dtsch. Akad. Wiss. Berlin, Jena, E. Ger.
SO Chem. Ber. (1971), 104(6), 1752-60
CODEN: CHBEAM

DT Journal
LA German
AB 2,3.beta.-Imino-5.alpha.-androstan-**17.beta.**-ol (I), prepd. from 2,3.alpha.-epoxyandrostan-17-one via the corresponding 2.beta.-azido-3.alpha.-tosyloxy compds., gave on reaction with HCl in Me2CO 3.alpha.-chloro-2.beta.-amino-5.alpha.-androstan-**17.beta.**-ol (II). Reaction of the diacetate of II with NaI and Me2CO gave **17.beta**.-acetoxy-2'-methyl-4',5'-dihydro-5.alpha.-**androst**-2-eno[2,3-d]oxazole (III, **17.beta.**-OAc), which on alk. hydrolysis yielded 2.beta.-amino-5.alpha.-androstane-3.beta.,-**17.beta.**-diol (IV) (R = OH), which was also obtained via the N-**phenylcarbamoyl** deriv. of I. Reaction of II with CS2 and alkali gave **17.beta**.-hydroxy-2'-thioxo-2',3',4'.alpha.,5'.alpha.-tetrahydro-5.alpha.-**androst**-2-eno[2.beta.,3.beta.-d]thiazole (V), which on sapon, with methanolic KOH under Ar yielded 2.beta.-amino-3.beta.-mercapto-5.alpha.-androstanol, IV (R = SH). The 2.beta.,3.alpha.-isomer of V was obtained from I.
IT Steroids, preparation
(from 2,3-imino derivs.)
IT 2639-53-4P 20793-31-1P 33210-98-9P 33211-00-6P 33211-02-8P 33211-03-9P 33211-04-0P 33211-05-1P 33211-06-2P 33211-07-3P 33267-13-9P 33267-14-0P 33294-40-5P 33294-41-6P 33294-42-7P 33397-55-6P
(prepn. of)

L13 ANSWER 5 OF 5 CA COPYRIGHT 1995 ACS DUPLICATE 5
AN 73:15117 CA
TI 2,3-Iminoandrostanes
IN Sasaki, Kanzo
PA Shionogi and Co., Ltd.
SO Japan., 4 pp.
CODEN: JAXXAD
PI JP 45006530 B4 700305 Showa
AI JP 661221
DT Patent
LA Japanese
AB **17.beta.**-Acetoxy-5.alpha.-**androst**-2-ene (22.07 g) in 200 ml Et2O is stirred 2 hr at 0.degree. with 15.7 g AgCN and 21.2 g iodine, stirred 38 hr at 3.degree. filtered, the filtrate concd., and the conc. refluxed 1 hr with 100 ml MeOH to give 18 g 2.beta.-(methoxyformamido)-3.alpha.-iodo-**17.beta.**-acetoxy-5.alpha.-androstane, m. 135-6.degree. (MeOH), and 11 g 2'-oxo-2.alpha.,3.alpha.-oxazolidino[4',5':2,3]-5.alpha.-androstan-**17.beta.**-ol acetate (I), m. 298-9.degree.. Similarly prepd. are 2.beta.-iodo-3.alpha.-(methoxyformamido)-**17.beta.**-acetoxy-5.alpha.-androstane, m. 199.degree. (decompn.). 2.alpha.,3.alpha.-imino-5.alpha.-androstan-**17.beta.**-ol (m. 202-3.degree.), and 2.alpha.,3.alpha.-(**phenylcarbamoylimino**)-5.alpha.-androstan-**17.beta.**-ol (m.200-1.degree.). The products are antiestrogenic, androgenic, and

anabolic agents.
IT Steroids, preparation
(2,3-imino)
IT 26737-08-6P 27510-00-5P 27510-01-6P 27601-47-4P 27727-62-4P
(prepn. of)

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FILE 'HOME' ENTERED AT 12:55:03 ON 03 NOV 95